

## Supplementary Information

# **Description of the Reaction Intermediate Stabilization for the Zimmerman Di- $\pi$ -methane Rearrangement on the Basis of a Parametric Diabatic Analysis**

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**Table S1.** Electronic energy +ZPE computed at M06-2X/ 6-31G(d) using PCM model with toluene.

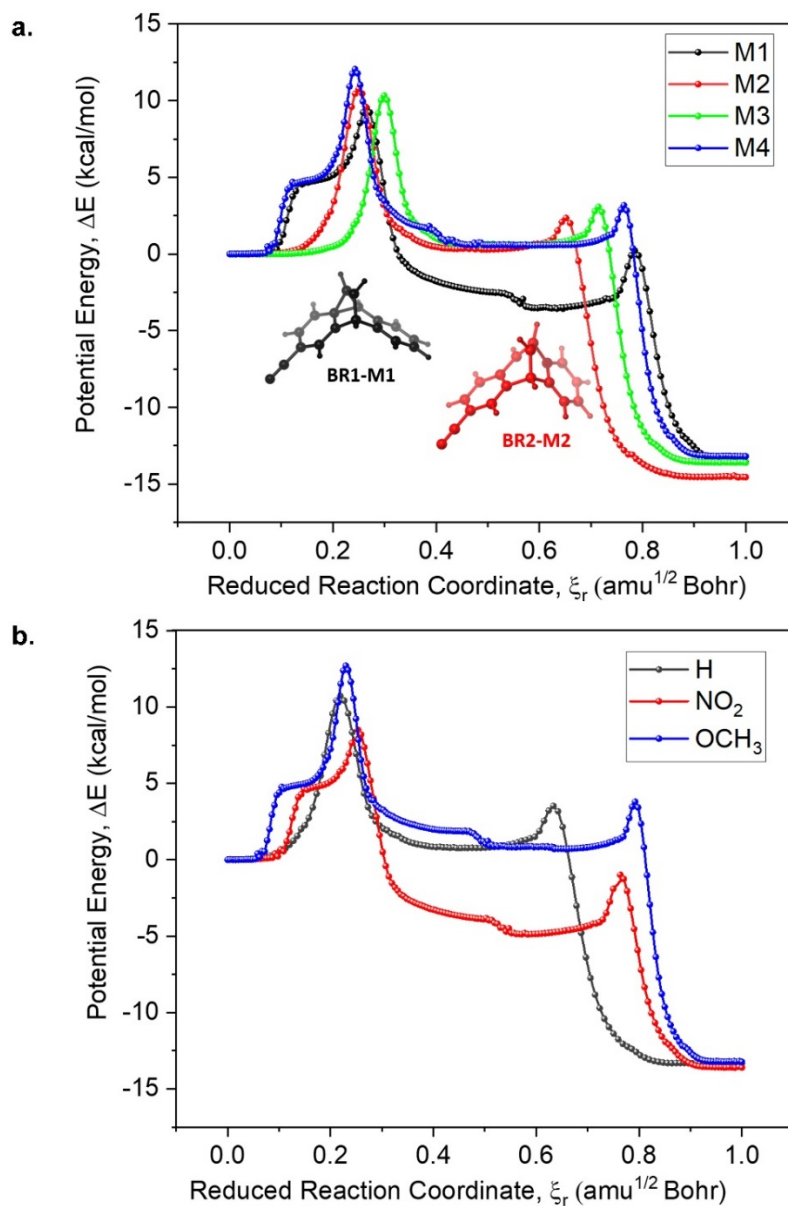
<b>Substituent</b>	<b>DBB*</b>	<b>TS1</b>	<b>BR1</b>	<b>TS2</b>	<b>BR2</b>
<b>H</b>	-616.31317	-616.29826	-616.31303	-616.30959	-616.33501
<b>CN-M1</b>	-708.53345	-708.52051	-708.53974	-708.53479	-708.55568
<b>CN-M2</b>	-708.53328	-708.51848	-708.53404	-708.53155	-708.55696
<b>CN-M3</b>	-708.53327	-708.51899	-708.53346	-708.53041	-708.55554
<b>CN-M4</b>	-708.53344	-708.51672	-708.5337	-708.53047	-708.55513
<b>NO<sub>2</sub>-M1</b>	-820.74099	-820.72974	-820.7492	-820.74412	-820.76322
<b>OCH<sub>3</sub>-M1</b>	-730.075826	-730.74032	-730.7581	-730.75415	-730.77983

**Table S2.** Enthalpies computed at M06-2X/ 6-31G(d) using PCM model with toluene.

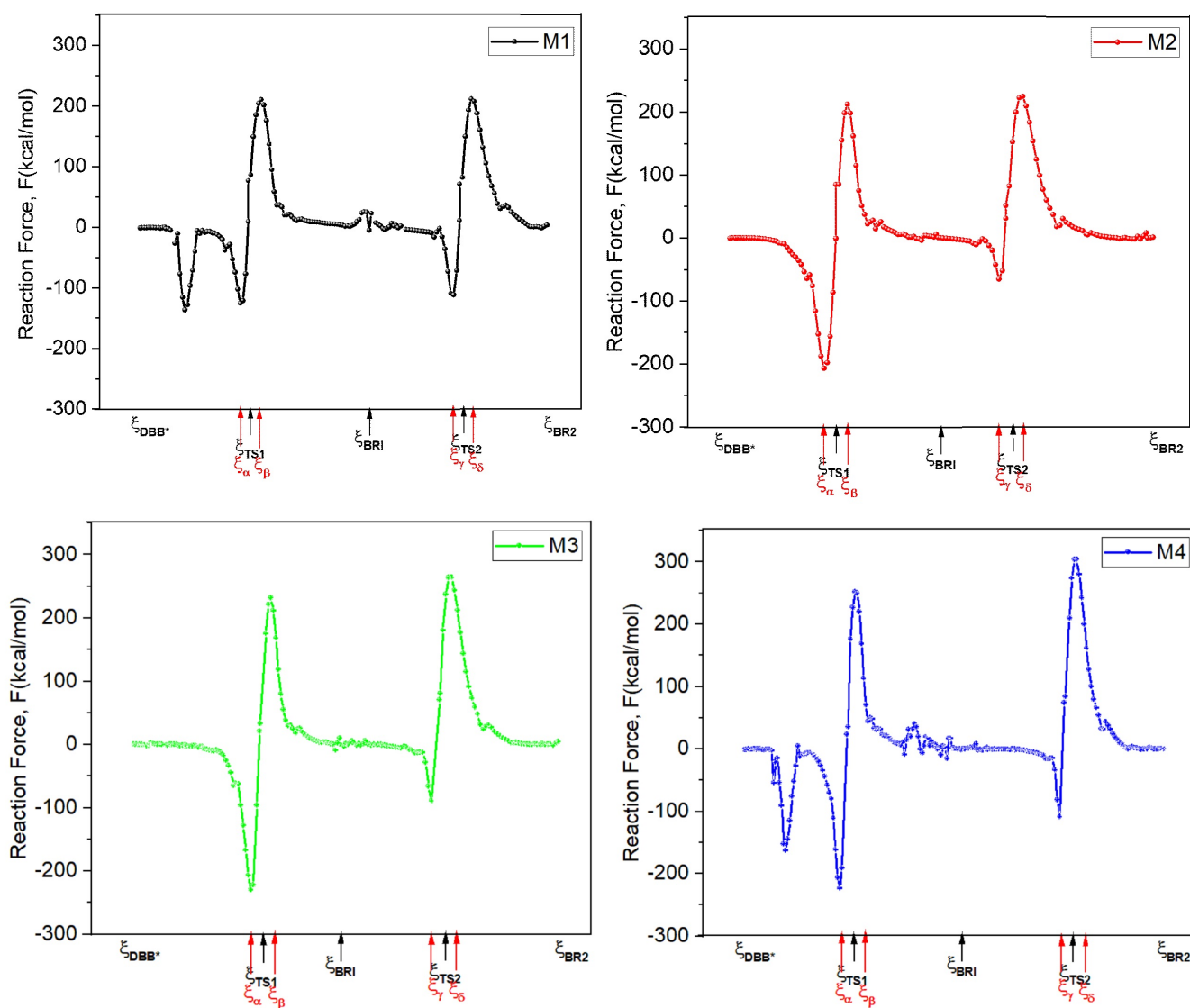
<b>Substituent</b>	<b>DBB*</b>	<b>TS1</b>	<b>BR1</b>	<b>TS2</b>	<b>BR2</b>
<b>H</b>	-616.30142	-616.28668	-616.30129	-616.29809	-616.32314
<b>CN-M1</b>	-708.51987	-708.50683	-708.52618	-708.52149	-708.54195
<b>CN-M2</b>	-708.51969	-708.50503	-708.52041	-708.51822	-708.54324
<b>CN-M3</b>	-708.51969	-708.50556	-708.51986	-708.51708	-708.54182
<b>CN-M4</b>	-708.51986	-708.50304	-708.5201	-708.51713	-708.54139
<b>NO<sub>2</sub>-M1</b>	-820.72669	-820.71534	-820.73498	-820.73014	-820.7488
<b>OCH<sub>3</sub>-M1</b>	-730.74394	-730.72595	-730.74375	-730.74009	-730.76541

**Table S3.** Gibbs free energies computed at M06-2X/ 6-31G(d) using PCM model with toluene.

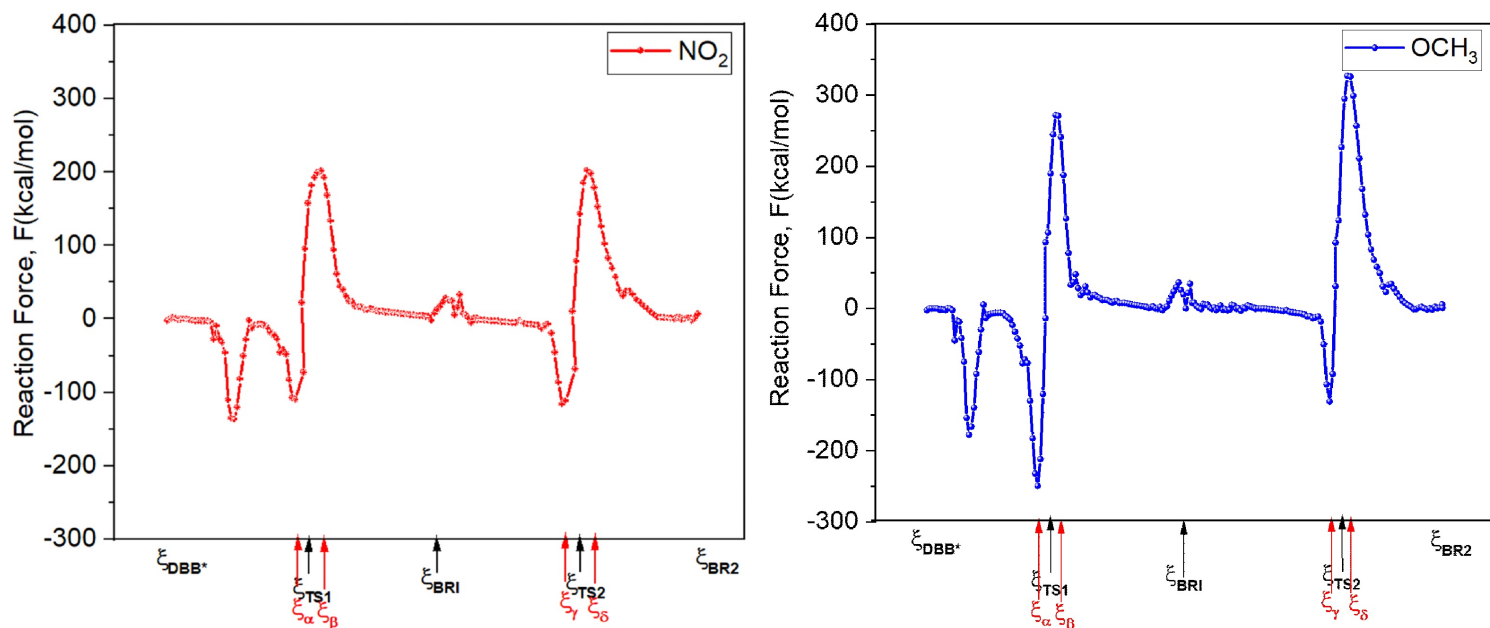
<b>Substituent</b>	<b>DBB*</b>	<b>TS1</b>	<b>BR1</b>	<b>TS2</b>	<b>BR2</b>
<b>H</b>	-616.3505	-616.33537	-616.35034	-616.34671	-616.37264
<b>CN-M1</b>	-708.57344	-708.56059	-708.57976	-708.57456	-708.59598
<b>CN-M2</b>	-708.57326	-708.55833	-708.57408	-708.57132	-708.59726
<b>CN-M3</b>	-708.57325	-708.55878	-708.57345	-708.57017	-708.59583
<b>CN-M4</b>	-708.57343	-708.55678	-708.57369	-708.57024	-708.59544
<b>NO<sub>2</sub>-M1</b>	-820.78248	-820.77123	-820.79048	-820.7852	-820.80495
<b>OCH<sub>3</sub>-M1</b>	-730.79896	-730.78103	-730.79888	-730.79459	-730.82078



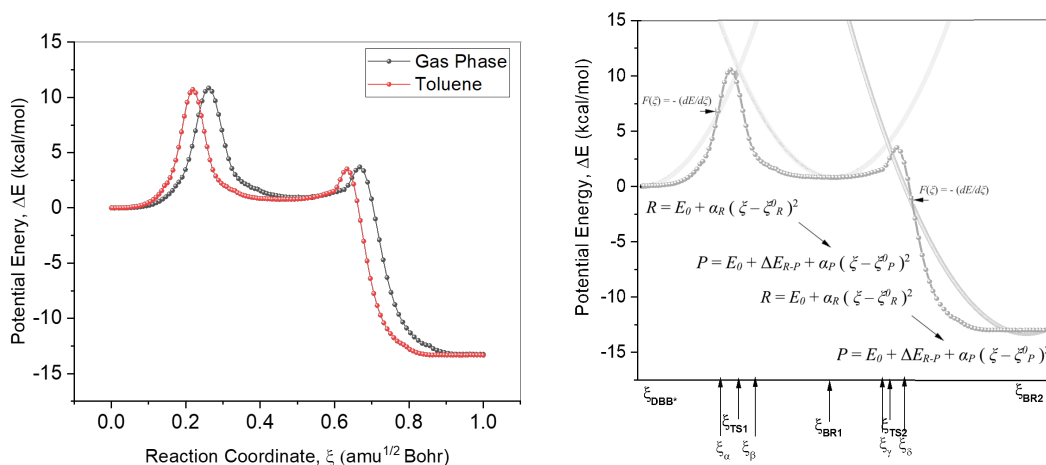
**Figure S1.** Potential energy surface along the reduced reaction coordinate for: (a) M1, M2, M3 and M4 reaction mechanisms substituted by CN and (b) unsubstituted (H)/substituted (NO<sub>2</sub>, OCH<sub>3</sub>) M1 reaction mechanisms.



**Figure S2.** Reaction force analysis along the reduced reaction coordinate for the M1, M2, M3 and M4 reaction mechanisms substituted by CN.  $\xi_{\text{DBB}^*}$ ,  $\xi_{\text{TS1}}$ ,  $\xi_{\text{BRI}}$ ,  $\xi_{\text{TS2}}$  and  $\xi_{\text{BR2}}$  denote the sites where each stationary point is located along the reaction coordinate.  $\{\xi_\alpha, \xi_\gamma\}$  denote the minimum and  $\{\xi_\beta, \xi_\delta\}$  the maximum of the reaction force.



**Figure S3.** Reaction force analysis along the reduced reaction coordinate for the M1 reaction mechanisms substituted by NO<sub>2</sub> and OCH<sub>3</sub>, respectively.  $\xi_{\text{DBB}^*}$ ,  $\xi_{\text{TS1}}$ ,  $\xi_{\text{BR1}}$ ,  $\xi_{\text{TS2}}$  and  $\xi_{\text{BR2}}$  denote the sites where each stationary point is located along the reaction coordinate.  $\{\xi_\alpha, \xi_\gamma\}$  denote the minimum and  $\{\xi_\beta, \xi_\delta\}$  the maximum of the reaction force.



**Figure S4. Left Panel:** IRC plot for the gas phase and the experimental solvent (toluene). **Right Panel:** The PDA of the IRC plot using the maximum gradients points (indicated by arrows on the IRC curve) from the Reaction Force Analysis (RFA). The vertex form of the quadratic functions modeling the parabolic wells are shown.  $\xi_{\text{DBB}^*}$ ,  $\xi_{\text{TS1}}$ ,  $\xi_{\text{BR1}}$ ,  $\xi_{\text{TS2}}$  and  $\xi_{\text{BR2}}$  denote the sites where each stationary point is located along the reaction coordinate.  $\{\xi_\alpha, \xi_\gamma\}$  denote the minimum and  $\{\xi_\beta, \xi_\delta\}$  the maximum of the reaction force.

## Optimized cartesian coordinates

### DBB\*-H

Electronic energy: -616.54217 Hartree

Lowest frequency: 69.4356 cm<sup>-1</sup>

C	-2.29233200	0.93777000	-2.59195200
C	-2.27834300	0.90332300	-1.19540100
C	-1.06948000	0.75181500	-0.52940900
C	0.13159000	0.65473700	-1.25234800
C	0.11453100	0.69387300	-2.63854800
C	-1.10391300	0.83296800	-3.30914800
C	-0.86489700	0.74037400	0.98295200
C	1.36218600	0.51589700	-0.37566000
C	1.11076400	-0.64765100	0.57959800
C	-0.07392900	-0.50903200	1.32252600
C	-0.42006300	-1.46552600	2.26524000
H	-1.33718800	-1.35838100	2.83857400
C	0.41843900	-2.56446400	2.47204100
C	1.59626600	-2.69641500	1.74192200
C	1.95022100	-1.73247600	0.79463600
H	-3.23536100	1.04585500	-3.11902400
H	-3.20437100	0.98766000	-0.63261300
H	1.04380900	0.61747800	-3.19705600
H	-1.12188100	0.86011800	-4.39426300
H	0.14927300	-3.31737700	3.20636000
H	2.24349700	-3.55218100	1.90786800
H	2.87059000	-1.83125100	0.22498300
H	-1.80928900	0.81187300	1.52875300
H	2.28467300	0.38921500	-0.94823500
C	1.39777100	1.69255400	0.59770700
C	0.04529200	1.95351200	1.16515000
H	-0.42770600	2.91669500	0.97483000
H	2.26034100	1.71385500	1.26346400

### TS1-H

Electronic energy: -616.52509 Hartree

Lowest frequency: -613.481 cm<sup>-1</sup>

C	-0.05114600	0.25703200	-0.04055800
C	-0.01422900	0.18319900	1.35312900
C	1.19943500	-0.01306000	1.99979600
C	2.38364200	-0.12947700	1.25460700
C	2.34400800	-0.05790500	-0.13202500
C	1.12246400	0.13616100	-0.77983300
C	1.40384200	-0.09338400	3.50490800

C	3.62957900	-0.34429900	2.06319400
C	3.44604700	-1.35501200	3.17548200
C	2.16714200	-1.35968700	3.82250700
C	1.86025100	-2.32073100	4.76030600
H	0.89990400	-2.29010500	5.26847400
C	2.79507900	-3.31893000	5.07330700
C	4.05429100	-3.31719600	4.45631600
C	4.39215800	-2.35627800	3.51974400
H	-0.99877200	0.40849600	-0.54826500
H	-0.92861200	0.27615600	1.93352800
H	3.26154600	-0.15235900	-0.70699800
H	1.08973600	0.19256000	-1.86341800
H	2.54859400	-4.08379500	5.80192200
H	4.77254400	-4.09290400	4.70555600
H	5.36022900	-2.37487900	3.02705900
H	0.46599200	0.00983500	4.05657800
H	4.54214000	-0.48638600	1.48422900
C	3.74883000	0.52944300	3.28123800
C	2.44529700	0.97255300	3.82475600
H	2.14887900	2.01930500	3.79698200
H	4.71414000	0.74439300	3.71920700

### BR1-H

Electronic energy: -616.54094 Hartree

Lowest frequency: 64.9525 cm<sup>-1</sup>

C	-2.39198400	0.98441200	-2.56257000
C	-2.31871300	1.00708700	-1.16864500
C	-1.09560000	0.82155100	-0.53815500
C	0.06970800	0.61619400	-1.29813500
C	-0.01093700	0.58720900	-2.68749700
C	-1.24145800	0.77299700	-3.31808100
C	-0.86925700	0.81121800	0.96927900
C	1.33012100	0.43567700	-0.54037200
C	1.23624200	-0.32922500	0.81546500
C	-0.15100500	-0.48313300	1.28932100
C	-0.55924100	-1.60517000	1.94326200
H	-1.58210300	-1.68983900	2.30122900
C	0.36498000	-2.65149700	2.18562700
C	1.72024900	-2.51250900	1.79624700
C	2.17695900	-1.39318600	1.15502900
H	-3.34788300	1.12933800	-3.05637800
H	-3.21416900	1.16583100	-0.57301400
H	0.88743700	0.42311300	-3.27693400
H	-1.29949400	0.75268100	-4.40195000
H	0.04118700	-3.55069900	2.69716500



H	2.41583400	-3.31510600	2.02434300
H	3.22008000	-1.29120400	0.86920400
H	-1.79502300	0.97269200	1.52665700
H	2.23789300	0.24440400	-1.10624900
C	1.49235400	1.18378500	0.77466300
C	0.23861000	1.81203100	1.24412600
H	0.07111200	2.88266400	1.25299900
H	2.46840200	1.58988000	1.01608800

### TS2-H

Electronic energy: -616.53656 Hartree

Lowest frequency: -543.3135 cm<sup>-1</sup>

C	0.00655900	0.01386700	0.01643400
C	0.00411400	-0.00257000	1.41273500
C	1.20330400	-0.00130100	2.11005800
C	2.43287500	0.02978700	1.41439200
C	2.42382300	0.01682800	0.01583700
C	1.21615300	0.01638800	-0.67675900
C	1.33462700	-0.09054200	3.62773000
C	3.65634400	0.03932200	2.20520500
C	3.55232200	-0.97237800	3.68420200
C	2.17169200	-1.32943100	3.89461400
C	1.81474100	-2.62080100	4.18578700
H	0.77009400	-2.88475100	4.32850000
C	2.81825100	-3.60050600	4.31906000
C	4.17308900	-3.25611300	4.16833800
C	4.56209100	-1.96314700	3.87746400
H	-0.93308200	0.01597100	-0.52701700
H	-0.93529900	-0.02631800	1.95968100
H	3.36610000	0.02303300	-0.52589400
H	1.21921000	0.01940400	-1.76242600
H	2.54562900	-4.62292300	4.55715500
H	4.93228600	-4.02102700	4.30277100
H	5.61173500	-1.69814000	3.78898700
H	0.35966600	-0.07588900	4.12138200
H	4.61661200	-0.07496700	1.71200900
C	3.64361400	0.53363800	3.62546000
C	2.29509600	1.00610100	4.04286900
H	4.53900200	1.03374300	3.98509500
H	2.01328400	2.05272700	4.04914800

### BR2-H

Electronic energy: -616.56341 Hartree

Lowest frequency: 62.8928 cm<sup>-1</sup>

C	-2.36688900	0.61662600	-2.58722400
C	-2.27995500	0.56762900	-1.19362300
C	-1.06542600	0.74558900	-0.55034300
C	0.11799200	0.99969300	-1.31349300
C	0.00605600	1.03148200	-2.72369800
C	-1.21617300	0.84568600	-3.34733300
C	-0.91639100	0.66121100	0.96812800
C	1.35563200	1.21996100	-0.65343900
C	1.24073600	-0.29781700	1.26352700
C	-0.12679100	-0.59766500	1.31046500
C	-0.56095300	-1.88273700	1.58970800
H	-1.62116600	-2.11927700	1.61954500
C	0.39563100	-2.87149100	1.84473100
C	1.75544800	-2.57216500	1.79946500
C	2.19180100	-1.27794800	1.49613800
H	-3.32500800	0.47344400	-3.07638800
H	-3.17193500	0.38162500	-0.60011300
H	0.89985100	1.21543000	-3.31435300
H	-1.28017800	0.88046100	-4.43056900
H	0.07488500	-3.88123400	2.08201500
H	2.48431800	-3.35085900	2.00273300
H	3.25304900	-1.04847700	1.45461500
H	-1.89209700	0.72427000	1.45839600
H	2.26822600	1.34067800	-1.22815400
C	1.39887500	1.17105900	0.86241100
C	0.08286300	1.72348200	1.35954400
H	2.29533800	1.65277200	1.26007200
H	-0.15060000	2.78260400	1.32630800

#### DBB\*-CN-M1

Electronic energy: -708.76116 Hartree

Lowest frequency: 48.9584 cm<sup>-1</sup>

C	-2.59823900	1.31752000	-2.86838900
C	-2.58895900	1.33630400	-1.47118400
C	-1.38433900	1.20958800	-0.79557900
C	-0.18547900	1.05924600	-1.51173600
C	-0.19335900	1.05317100	-2.90013300
C	-1.40840600	1.17780300	-3.57767000
C	-1.20049300	1.21849800	0.71086400
C	1.04776300	0.98228400	-0.61570400
C	0.81026500	-0.13877600	0.37680000
C	-0.40645300	-0.03049000	1.07608000
C	-0.75567400	-0.97211400	2.03627500
H	-1.69109100	-0.87920300	2.58005200
C	0.09755600	-2.04307400	2.29153000

C	1.30108200	-2.15266500	1.58901500
C	1.66556900	-1.19558900	0.62818700
H	-3.53861400	1.41302100	-3.40206800
H	-3.51625200	1.45038500	-0.91611300
H	0.73712800	0.94639900	-3.45124600
H	-1.42357200	1.16420800	-4.66303500
H	-0.16297700	-2.79418600	3.02941400
H	2.60747200	-1.29148700	0.09665400
H	-2.14316600	1.28370600	1.25962000
H	1.97062100	0.85898900	-1.18753100
C	0.95588700	2.31153000	0.13142900
C	-0.19736900	2.31157000	1.07367100
H	-0.00954700	2.43560400	2.13960600
H	1.13630100	3.19475400	-0.48013800
C	2.18087800	-3.25936500	1.85493200
N	2.89025900	-4.14907000	2.06873100

### TS1-CN-M1

Electronic energy: -708.74595 Hartree

Lowest frequency: -590.43 cm<sup>-1</sup>

C	0.00166400	0.21410700	-0.13156400
C	0.01514400	0.15567800	1.26257700
C	1.22140500	-0.02354500	1.92796600
C	2.41544800	-0.14633100	1.20519600
C	2.40043300	-0.08711400	-0.18236400
C	1.18853800	0.09320500	-0.85037600
C	1.37599500	-0.12025900	3.42126900
C	3.64865100	-0.32291300	2.06627000
C	3.42662200	-1.46843300	3.03214400
C	2.25533200	-1.27860600	3.83197900
C	2.01419800	-2.14054600	4.92850400
H	1.12584000	-2.00296900	5.53777500
C	2.88831400	-3.16865900	5.19514300
C	4.04312700	-3.35210100	4.39492100
C	4.31812300	-2.48084000	3.33062200
H	-0.93832400	0.35279700	-0.65632400
H	-0.90936900	0.24822400	1.82626000
H	3.32821400	-0.18098800	-0.74042800
H	1.17210700	0.13907500	-1.93477100
H	2.69769200	-3.85565200	6.01272600
H	5.22544000	-2.60670800	2.74719700
H	0.44327200	-0.06791600	3.98282100
H	4.56628500	-0.42021800	1.48404100
C	3.67894700	0.81639200	3.07180300
C	2.48280800	0.72803800	3.96458900

H	2.49765000	1.01931500	5.00636900
H	4.61896300	1.20367400	3.44588700
C	4.94166600	-4.42884600	4.68183900
N	5.67193000	-5.29848100	4.91732900

### BR1-CN-M1

Electronic energy: -708.76682 Hartree

Lowest frequency: 41.1398 cm<sup>-1</sup>

C	-2.55993900	1.05735200	-2.96845500
C	-2.60262900	1.04306500	-1.57397500
C	-1.41808500	1.08346800	-0.84534100
C	-0.18584200	1.12789100	-1.51882800
C	-0.14572900	1.14369500	-2.90625900
C	-1.33738300	1.10956200	-3.63277100
C	-1.36277000	1.08723700	0.63705400
C	1.02946400	1.15540600	-0.59818800
C	0.88548700	-0.02304900	0.34271900
C	-0.18010900	0.31678700	1.29833400
C	-0.40430200	-0.59639200	2.41171400
H	-1.15068900	-0.34992600	3.16104700
C	0.29881200	-1.76009100	2.48106300
C	1.28984200	-2.08393900	1.50361400
C	1.59112500	-1.17609200	0.44253300
H	-3.48502500	1.02733800	-3.53541100
H	-3.55655500	1.00399200	-1.05479600
H	0.81161100	1.17867600	-3.41961500
H	-1.30870700	1.12020400	-4.71779200
H	0.12242900	-2.46038800	3.29079500
H	2.39355300	-1.41009500	-0.25034200
H	-2.30150500	1.01475400	1.17907600
H	1.97005000	1.18509700	-1.15204900
C	0.80897100	2.30007100	0.37291800
C	-0.24365200	1.85441900	1.31215100
H	-0.46357500	2.38677800	2.23072600
H	0.97735600	3.33711900	0.10954100
C	2.00783100	-3.30567000	1.61128300
N	2.59559900	-4.30464900	1.69872900

### TS2-CN-M1

Electronic energy: -708.7608 Hartree

Lowest frequency: -529.4373 cm<sup>-1</sup>

C	-2.41478900	0.89324000	-3.01785000
C	-2.53849100	0.95861900	-1.63295700
C	-1.39957100	1.10159200	-0.83337200

C	-0.12612500	1.13194000	-1.44458400
C	-0.01100800	1.06464700	-2.82462900
C	-1.15685600	0.95283700	-3.61548200
C	-1.45833900	1.19836200	0.61688800
C	1.04754200	1.17908700	-0.47028500
C	0.88110100	-0.03267300	0.43132200
C	-0.08764300	0.30301500	1.43993500
C	-0.45050700	-0.66626200	2.41752700
H	-1.13857400	-0.41025000	3.21722900
C	0.08844800	-1.92985200	2.32995900
C	1.01254300	-2.25767500	1.31061500
C	1.41156000	-1.28860000	0.35431700
H	-3.30362800	0.79517200	-3.63296200
H	-3.51927500	0.91663500	-1.16694100
H	0.97355400	1.08770000	-3.28454600
H	-1.06484900	0.90128700	-4.69566500
H	-0.17675200	-2.68736800	3.05996700
H	2.13671400	-1.55163700	-0.40980500
H	-2.39728800	1.02356100	1.13283100
H	2.00652700	1.23777200	-0.99010600
C	0.75737200	2.30576800	0.49973500
C	-0.32022900	1.79394800	1.39254600
H	-0.57203700	2.32146500	2.30901200
H	0.84778600	3.34970500	0.22449200
C	1.56416800	-3.57374400	1.25534500
N	2.01246900	-4.64327900	1.20861600

### BR2-CN-M1

Electronic energy: -708.78275 Hartree

Lowest frequency: 45.8798 cm<sup>-1</sup>

C	-2.33578400	1.08889300	-3.09124900
C	-2.52759900	1.34067000	-1.74349400
C	-1.43057900	1.41244200	-0.85258600
C	-0.11963700	1.19328100	-1.38075400
C	0.05216500	0.94680200	-2.73348200
C	-1.04617900	0.89448500	-3.59517000
C	-1.60340000	1.69992300	0.52675500
C	1.04704600	1.22036700	-0.39366300
C	0.93349300	0.00275200	0.51548200
C	0.10111700	0.32335100	1.59858500
C	-0.21103900	-0.61903700	2.56627100
H	-0.85957700	-0.37278200	3.40137700
C	0.33722300	-1.89681200	2.45637700
C	1.16631600	-2.21379200	1.37483000
C	1.46607600	-1.26399500	0.38258300

H	-3.19056700	1.04431900	-3.75888600
H	-3.52948700	1.49711600	-1.35224300
H	1.05511100	0.78738200	-3.12182200
H	-0.89679700	0.69918600	-4.65206100
H	0.12839900	-2.65237300	3.20612000
H	2.10580100	-1.53139900	-0.45273600
H	-2.59894800	1.79567600	0.94731800
H	2.00273500	1.29668800	-0.91911900
C	0.75184100	2.32303700	0.59425400
C	-0.38038500	1.76364900	1.42374000
H	-0.58734900	2.28490500	2.36095400
H	0.81469500	3.37330800	0.33162500
C	1.72556300	-3.53601500	1.27912800
N	2.17647100	-4.59962100	1.20111400

### DBB\*-CN-M2

Electronic energy: -708.761 Hartree

Lowest frequency: 48.8178 cm<sup>-1</sup>

C	-2.61605600	1.25711300	-2.87006600
C	-2.60134000	1.28226400	-1.47361400
C	-1.38931700	1.17516000	-0.80477700
C	-0.18831700	1.06220900	-1.52419300
C	-0.20602100	1.04096000	-2.91074900
C	-1.42687300	1.13662500	-3.58391400
C	-1.18513500	1.23394500	0.70723100
C	1.04539600	0.97698000	-0.64459200
C	0.80502500	-0.14666900	0.35833100
C	-0.38216400	0.00966000	1.09784600
C	-0.72269600	-0.90822300	2.08125300
H	-1.63963300	-0.78582100	2.65006200
C	0.11822300	-1.98967500	2.33811700
C	1.30036100	-2.13590600	1.60708600
C	1.65433700	-1.20952700	0.61390500
H	-3.56055000	1.33100900	-3.40008300
H	-3.52763300	1.37906300	-0.91361100
H	0.72340200	0.95182900	-3.46673600
H	-1.44640300	1.11704500	-4.66901700
H	-0.13466400	-2.71831300	3.10058700
H	2.57792100	-1.33505100	0.05699900
H	-2.12914100	1.31778600	1.25106200
H	1.96914000	0.83453200	-1.21059600
C	1.06855300	2.19257900	0.27949800
C	-0.28591400	2.46249900	0.83722500
H	-0.77155500	3.40976500	0.60570100
H	1.93367100	2.25882000	0.93834500

C	2.16863800	-3.25156100	1.87599400
N	2.86906300	-4.14777200	2.09165900

### TS1-CN-M2

Electronic energy: -708.74384 Hartree

Lowest frequency: -616.2711 cm<sup>-1</sup>

C	0.04478300	0.32157800	-0.06005600
C	0.07562600	0.32881700	1.32296600
C	1.29104200	0.02975000	1.99281100
C	2.45840200	-0.26025900	1.21487100
C	2.40378600	-0.24910300	-0.16173800
C	1.19169000	0.02560900	-0.81107800
C	1.42207700	-0.14320500	3.49180000
C	3.68708800	-0.31433600	2.09507800
C	3.49009100	-1.41137600	3.12871800
C	2.29988500	-1.29762600	3.86872800
C	1.99653100	-2.22549400	4.85815800
H	1.07407300	-2.13681900	5.42430200
C	2.87869700	-3.26900800	5.12433700
C	4.06439900	-3.37457700	4.39111300
C	4.37523800	-2.44465600	3.38841700
H	-0.88899200	0.53392300	-0.57221900
H	-0.82148200	0.53494700	1.89971600
H	3.30555400	-0.43546700	-0.73885900
H	1.14445600	0.02159100	-1.89463500
H	2.65606000	-3.99948900	5.89435800
H	5.29916500	-2.54034100	2.82591600
H	0.47613400	-0.08407700	4.02942200
H	4.62478700	-0.42692200	1.54589300
C	3.56005100	0.99124900	2.87064600
C	2.14793300	1.15708000	3.28021500
H	1.62940600	2.10110600	3.37591200
H	4.37834400	1.30284300	3.51610400
C	4.97926100	-4.45023700	4.66826500
N	5.71707700	-5.31430900	4.89030000

### BR1-CN-M2

Electronic energy: -708.76051 Hartree

Lowest frequency: 46.8885 cm<sup>-1</sup>

C	-2.60161600	1.46014600	-2.75076700
C	-2.50010600	1.82427800	-1.43590800
C	-1.25582400	1.56433200	-0.71755900
C	-0.13237900	1.01307000	-1.49554100
C	-0.27017000	0.68273800	-2.80906500

C	-1.51661300	0.87856000	-3.45262100
C	-1.27086700	1.06142700	0.76386100
C	1.07080300	0.99787500	-0.57538300
C	0.84070200	-0.14025700	0.41019500
C	-0.39386900	-0.08201000	1.08720100
C	-0.73178700	-1.07955300	1.99982700
H	-1.68589600	-1.03933400	2.51694600
C	0.15188900	-2.12238700	2.25453700
C	1.38025600	-2.16741900	1.58672600
C	1.72634500	-1.17455300	0.65866500
H	-3.53564200	1.63016300	-3.27827500
H	-3.33305200	2.27988400	-0.90823900
H	0.57618000	0.29464000	-3.36955600
H	-1.63335500	0.60862700	-4.49581800
H	-0.10133100	-2.89996900	2.96690000
H	2.67986300	-1.22368300	0.14119700
H	-2.24064000	1.10938100	1.25081100
H	2.03635700	0.91791400	-1.07950300
C	0.84136000	2.28422700	0.19674400
C	-0.61858100	2.39019900	0.40328900
H	-1.08768300	3.29858600	0.76398400
H	1.57833400	2.70764100	0.86831700
C	2.29818900	-3.24235600	1.85127300
N	3.03932900	-4.10646800	2.06321500

## TS2-CN-M2

Electronic energy: -708.75724 Hartree

Lowest frequency: -523.8852 cm<sup>-1</sup>

C	-2.55826000	1.24622000	-2.81028400
C	-2.47789200	1.79154600	-1.54521100
C	-1.24584400	1.67814400	-0.82870900
C	-0.10534200	1.08698600	-1.48603700
C	-0.21393000	0.55539100	-2.74449000
C	-1.45014100	0.62639800	-3.41634500
C	-1.32639900	1.06844900	0.83812200
C	1.04881500	1.10788800	-0.49937500
C	0.80494200	-0.07654700	0.42935700
C	-0.45559300	-0.06976400	1.07492700
C	-0.82333500	-1.16136000	1.87153600
H	-1.79666100	-1.17111200	2.35319300
C	0.05558600	-2.21668900	2.06520000
C	1.31276000	-2.19893200	1.44633900
C	1.68209100	-1.12776900	0.61776500
H	-3.49285600	1.31324900	-3.35890400
H	-3.32876900	2.29172000	-1.09215300



H	0.64607900	0.09913200	-3.22712300
H	-1.54395300	0.21559200	-4.41555400
H	-0.22044300	-3.05585400	2.69448600
H	2.64886800	-1.13476600	0.12271300
H	-2.34554200	1.04859000	1.21064700
H	2.04412300	1.07518100	-0.94856000
C	0.72881700	2.35602000	0.29828500
C	-0.75448800	2.39186200	0.40748500
H	-1.26417300	3.28642400	0.75378300
H	1.38964300	2.74738800	1.06240500
C	2.22666700	-3.28767800	1.65050400
N	2.96553200	-4.16492900	1.81372300

## BR2-CN-M2

Electronic energy: -708.78418 Hartree

Lowest frequency: 45.4251 cm<sup>-1</sup>

C	-2.41308100	1.29399800	-2.99621200
C	-2.39125500	1.88916900	-1.73031700
C	-1.23019000	1.79831800	-0.98024100
C	-0.11137400	1.11062300	-1.46584400
C	-0.13733900	0.50270100	-2.70978900
C	-1.30080700	0.60842000	-3.47961900
C	-1.23887000	1.14140100	1.37171100
C	0.98389300	1.14418200	-0.40426400
C	0.76991600	-0.02823900	0.55017500
C	-0.38626500	0.01544900	1.39929300
C	-0.63264800	-1.08680000	2.25722700
H	-1.51031900	-1.06737000	2.89678600
C	0.22563600	-2.16493300	2.29898600
C	1.36441600	-2.18154100	1.47427700
C	1.62556100	-1.10925000	0.60321400
H	-3.30644000	1.36819200	-3.60857700
H	-3.26200500	2.41792100	-1.35299000
H	0.72729700	-0.03704900	-3.08601300
H	-1.33617100	0.15295100	-4.46434500
H	0.03332600	-3.00056200	2.96317300
H	2.50452400	-1.14028800	-0.03436900
H	-2.14721700	1.15148500	1.96546700
H	2.00026000	1.13717400	-0.80721100
C	0.58872700	2.38789500	0.35528700
C	-0.91677300	2.29048900	0.43594500
H	-1.43764900	3.20647100	0.72296500
H	1.19081300	2.80173200	1.15697200
C	2.26226800	-3.29818800	1.51737500
N	2.98923400	-4.20022100	1.55159600

**DBB\*-CN-M3**

Electronic energy: -708.761 Hartree

Lowest frequency: 48.9397 cm<sup>-1</sup>

C	-2.59220500	1.30202900	-2.87210500
C	-2.58549300	1.31244400	-1.47542100
C	-1.37801400	1.19116600	-0.80075900
C	-0.17354300	1.07873600	-1.51440600
C	-0.18326400	1.07221900	-2.90121400
C	-1.39959500	1.18204000	-3.58034300
C	-1.18232300	1.23311000	0.71293800
C	1.05451600	0.97725800	-0.62863200
C	0.80196700	-0.15516900	0.36129700
C	-0.38861500	0.00029900	1.09553700
C	-0.73997800	-0.92564400	2.06754000
H	-1.65951200	-0.80388600	2.63228100
C	0.09340900	-2.01433500	2.31822200
C	1.27897600	-2.15973000	1.59258700
C	1.64385500	-1.22529300	0.61096400
H	-3.53313700	1.38706900	-3.40676800
H	-3.51447000	1.40877300	-0.91979600
H	0.74885800	0.98352500	-3.45275400
H	-1.41296400	1.17403700	-4.66569300
H	-0.16797000	-2.74922800	3.07178800
H	2.56993300	-1.35037600	0.05811500
H	-2.12899200	1.31681400	1.25214000
H	1.98068900	0.83531900	-1.19079600
C	1.07921500	2.18321100	0.30797000
C	-0.27689900	2.45507000	0.86077500
H	-0.75582700	3.40744100	0.63612100
H	1.94095400	2.23801200	0.97228700
C	2.13949000	-3.28285100	1.85524500
N	2.83372600	-4.18505300	2.06597100

**TS1-CN-M3**

Electronic energy: -708.74452 Hartree

Lowest frequency: -605.8265 cm<sup>-1</sup>

C	-0.04847800	0.25029200	-0.03515400
C	-0.01049800	0.17422800	1.35814700
C	1.20514200	-0.01966300	2.00163900
C	2.38795900	-0.13215900	1.25493600
C	2.34767900	-0.05860000	-0.13145200
C	1.12452900	0.13365400	-0.77628600
C	1.41002200	-0.10075100	3.50712800

C	3.63643400	-0.34430000	2.06125200
C	3.45167800	-1.35960900	3.17098800
C	2.17356000	-1.36587300	3.82271000
C	1.86334500	-2.32658000	4.76025400
H	0.90398000	-2.29652300	5.26846700
C	2.79002000	-3.32665900	5.07680600
C	4.05151100	-3.31721700	4.45293200
C	4.39759200	-2.35589300	3.50997300
H	-0.99691700	0.40012500	-0.54150200
H	-0.92422000	0.26395700	1.93976000
H	3.26443200	-0.15025000	-0.70777300
H	1.08988600	0.19154000	-1.85957500
H	2.55517500	-4.09504300	5.80377900
H	5.36862300	-2.38577600	3.02626700
H	0.47371800	0.00113600	4.06071900
H	4.54876000	-0.48703900	1.48266200
C	3.75615600	0.52621400	3.27902900
C	2.45276900	0.96278300	3.82919200
H	2.15760900	2.00936000	3.81383900
H	4.72097800	0.74046000	3.71882700
C	5.00706100	-4.34311600	4.78582300
N	5.77551500	-5.16599100	5.05529500

### BR1-CN-M3

Electronic energy: -708.76006 Hartree

Lowest frequency: 48. 646 cm<sup>-1</sup>

C	-2.72259500	1.38201100	-2.81934900
C	-2.65363300	1.41918000	-1.42570600
C	-1.42972500	1.25103700	-0.79209000
C	-0.26216800	1.04751500	-1.54769700
C	-0.33806200	1.00301100	-2.93672000
C	-1.56892300	1.17266000	-3.57072500
C	-1.20768700	1.25719300	0.71675400
C	0.99992000	0.88751200	-0.78692700
C	0.90139300	0.12612900	0.57519700
C	-0.48600100	-0.03163300	1.04648100
C	-0.89672000	-1.15293400	1.70247100
H	-1.92007900	-1.24093900	2.05560400
C	0.02100800	-2.19717000	1.95346900
C	1.38115900	-2.04547100	1.56466400
C	1.84577700	-0.92374900	0.91931500
H	-3.67845400	1.51371600	-3.31662300
H	-3.55163800	1.57591200	-0.83376900
H	0.56265500	0.83993900	-3.52247300
H	-1.62496900	1.14077100	-4.65422100

H	-0.28896900	-3.10007200	2.46459800
H	2.89229300	-0.83039900	0.64746900
H	-2.13504500	1.41724100	1.27103900
H	1.90955400	0.69193500	-1.34793100
C	1.15379900	1.64145100	0.52094300
C	-0.10464700	2.26300900	0.98832800
H	-0.27490900	3.33258300	1.00375000
H	2.12751800	2.04848400	0.76939400
C	2.30933200	-3.10384400	1.87441300
N	3.05171900	-3.95601600	2.12474200

### TS2-CN-M3

Electronic energy: -708.7561 Hartree

Lowest frequency: -528.5964 cm<sup>-1</sup>

C	0.01406200	-0.00229500	0.02299100
C	0.01035800	-0.01561400	1.41902900
C	1.21034500	-0.00707900	2.11513600
C	2.43824400	0.02519700	1.41841100
C	2.43094800	0.00853300	0.02016700
C	1.22300600	0.00309800	-0.67145500
C	1.34104000	-0.09144200	3.63383900
C	3.66356700	0.04311000	2.20746400
C	3.55846100	-0.97081100	3.68243200
C	2.17694700	-1.33076800	3.89573500
C	1.81584500	-2.62202900	4.18384400
H	0.77212500	-2.88525900	4.32847300
C	2.80984600	-3.60709600	4.31136400
C	4.16817000	-3.25317300	4.15751200
C	4.56770500	-1.95544100	3.87177000
H	-0.92555200	-0.00509000	-0.52027100
H	-0.92897500	-0.04125800	1.96555100
H	3.37312400	0.01564000	-0.52130000
H	1.22502400	0.00335300	-1.75689300
H	2.54887200	-4.63253600	4.54392600
H	5.62024100	-1.70459200	3.78998600
H	0.36686800	-0.07891300	4.12811700
H	4.62380800	-0.07014200	1.71387500
C	3.65032000	0.53615500	3.62672100
C	2.30182700	1.00372700	4.04923600
H	4.54654200	1.03245700	3.98867600
H	2.01975700	2.04951900	4.06999200
C	5.17568400	-4.26896300	4.32923600
N	5.98414300	-5.08625800	4.46632500

### BR2-CN-M3

Electronic energy: -708.78266 Hartree

Lowest frequency: 43.7381 cm<sup>-1</sup>

C	-2.77088600	1.06899800	-2.74795500
C	-2.66163900	0.98778100	-1.35781200
C	-1.44115400	1.18052700	-0.73033500
C	-0.27604600	1.48062800	-1.50386300
C	-0.41065800	1.54406800	-2.91118200
C	-1.63788800	1.34426800	-3.51972700
C	-1.26816100	1.06425100	0.78443200
C	0.96692200	1.71190200	-0.85840800
C	0.91158100	0.14227400	1.01356500
C	-0.45070000	-0.18790600	1.07387100
C	-0.86103500	-1.48844600	1.31890800
H	-1.91532600	-1.74529500	1.35770900
C	0.10882900	-2.46920300	1.52852100
C	1.46610800	-2.13519500	1.47034800
C	1.88417200	-0.82062000	1.19998100
H	-3.73285400	0.91508200	-3.22602900
H	-3.53967400	0.76668600	-0.75575200
H	0.46904500	1.76327600	-3.51055800
H	-1.72022100	1.40371600	-4.60047100
H	-0.17892000	-3.49346400	1.73960400
H	2.94244100	-0.58415400	1.15166500
H	-2.23648700	1.09092700	1.29135800
H	1.86780900	1.87047300	-1.44176100
C	1.03510400	1.62401000	0.65534800
C	-0.28303200	2.13344700	1.19053100
H	1.92880500	2.10927400	1.05355100
H	-0.53768300	3.18753300	1.19849300
C	2.45431100	-3.15731200	1.69344200
N	3.25166200	-3.97765500	1.87182800

#### **DBB\*-CN-M4**

Electronic energy: -708.76116 Hartree

Lowest frequency: 49.0279 cm<sup>-1</sup>

C	-2.59216700	1.32166100	-2.87405400
C	-2.59110700	1.32882300	-1.47670900
C	-1.38948500	1.20567200	-0.79516100
C	-0.18539700	1.07042000	-1.50551700
C	-0.18518300	1.07587300	-2.89396100
C	-1.39721900	1.19690200	-3.57751900
C	-1.21429900	1.20367700	0.71240000
C	1.04326700	0.99555000	-0.60295400
C	0.80871700	-0.13518600	0.37910400

C	-0.41281900	-0.04198500	1.07210300
C	-0.76033400	-0.99419300	2.02243000
H	-1.69965800	-0.91300900	2.56131500
C	0.09975100	-2.06050000	2.27410000
C	1.30835600	-2.15481500	1.57809400
C	1.67091100	-1.18719100	0.62717700
H	-3.53014800	1.41447400	-3.41239900
H	-3.52247300	1.43115200	-0.92617500
H	0.74925500	0.98072900	-3.44048200
H	-1.40600000	1.19231400	-4.66302200
H	-0.15920300	-2.81964000	3.00427800
H	2.61674300	-1.27119600	0.10065000
H	-2.16054600	1.25732600	1.25622000
H	1.97024700	0.88384700	-1.17048700
C	0.93674500	2.31812900	0.15407000
C	-0.22184400	2.30156600	1.08968000
H	-0.04117000	2.41891300	2.15763200
H	1.11353800	3.20755400	-0.44951700
C	2.19541900	-3.25658500	1.84036100
N	2.91106300	-4.14206900	2.05076600

#### TS1-CN-M4

Electronic energy: -708.74194 Hartree

Lowest frequency: -578.3637 cm<sup>-1</sup>

C	0.01585200	0.23946900	-0.00021800
C	-0.00306800	0.03869400	1.37771800
C	1.18478100	-0.17185400	2.06353500
C	2.43712600	-0.13043500	1.36649500
C	2.44023800	0.10051700	-0.03412100
C	1.24364700	0.27386700	-0.69495500
C	1.38459500	-0.17966400	3.56363800
C	3.66403800	-0.38195400	2.20924600
C	3.44998900	-1.45512900	3.23622500
C	2.24204600	-1.36430400	3.94586500
C	1.92102800	-2.31206800	4.91057600
H	0.98551400	-2.23715200	5.45705800
C	2.80102500	-3.35696500	5.17536300
C	4.00287500	-3.44432800	4.46547900
C	4.33246700	-2.49270100	3.49032000
H	-0.91430000	0.37188400	-0.54244200
H	-0.94393700	0.04167800	1.92191200
H	3.38308400	0.11689100	-0.57362200
H	1.24357700	0.42770900	-1.76979600
H	2.56526700	-4.10381800	5.92567200
H	5.26856800	-2.57474600	2.94626100

H	0.45239500	-0.13109700	4.12868700
H	4.58144400	-0.47892900	1.62963600
C	3.35959700	1.00149100	2.69302000
C	2.24046700	1.07526700	3.67644100
H	1.77481300	2.02773200	3.90205400
H	3.80648800	1.86546300	2.22182000
C	4.91384600	-4.52437700	4.73770700
N	5.64802800	-5.39261700	4.95559600

#### BR1-CN-M4

Electronic energy: -708.76026 Hartree

Lowest frequency: 46.6046 cm<sup>-1</sup>

C	-2.51277600	0.98760700	-2.84147800
C	-2.55537300	0.89843100	-1.42858300
C	-1.42725000	1.13905800	-0.70537400
C	-0.15091700	1.48197800	-1.35761300
C	-0.16746800	1.64199500	-2.80919800
C	-1.31781500	1.37326600	-3.49895100
C	-1.18773700	1.20581800	0.78911300
C	1.08487500	0.87137400	-0.62592300
C	0.81084200	-0.17313900	0.38517900
C	-0.36560000	-0.02435200	1.14600000
C	-0.69691000	-0.95568200	2.12265600
H	-1.60578000	-0.83066300	2.70413600
C	0.13258800	-2.04920200	2.35275800
C	1.29587000	-2.20111100	1.59134900
C	1.63776500	-1.26616900	0.60511200
H	-3.40614400	0.78838700	-3.42195700
H	-3.49040700	0.66471700	-0.92632400
H	0.74097300	1.94769600	-3.32019100
H	-1.32251300	1.46733100	-4.58095500
H	-0.11365600	-2.78345400	3.11198100
H	2.54553100	-1.39972900	0.02453200
H	-2.09073900	1.28922500	1.39786400
H	1.97139700	0.75774600	-1.24318200
C	0.63726500	2.29504100	-0.32420400
C	-0.23928100	2.38895000	0.86207000
H	0.05633200	2.84981900	1.79678400
H	1.28609200	3.10804600	-0.62973400
C	2.15651000	-3.33038100	1.82370300
N	2.85039000	-4.23819800	2.01061700

#### TS2-CN-M4

Electronic energy: -708.75609 Hartree

Lowest frequency: -535.4802 cm<sup>-1</sup>

C	-2.47232100	0.66931600	-2.82974200
C	-2.49474800	0.77116000	-1.42565000
C	-1.37825100	1.22241300	-0.76942100
C	-0.17512700	1.54976000	-1.49222300
C	-0.18518000	1.49203300	-2.91926700
C	-1.32289500	1.03489400	-3.55348900
C	-1.07695700	1.37494500	0.71166100
C	1.21555800	0.79616600	-0.65146100
C	0.81217400	-0.17926000	0.34981700
C	-0.35261400	0.09410900	1.10701500
C	-0.78539100	-0.79391100	2.08237300
H	-1.67965900	-0.56915300	2.65689200
C	-0.08562300	-1.97393300	2.31851800
C	1.04975900	-2.26095000	1.55052100
C	1.49658800	-1.37535700	0.56511700
H	-3.35329200	0.32257400	-3.35863100
H	-3.39308800	0.51139200	-0.87209700
H	0.69094300	1.79643600	-3.48422900
H	-1.33784400	0.97327400	-4.63744800
H	-0.41270900	-2.67272800	3.08040400
H	2.38136100	-1.61554900	-0.01656400
H	-1.94678100	1.56253800	1.34559300
H	2.02053900	0.55842800	-1.33920100
C	0.77613500	2.22981200	-0.53741100
C	-0.03321200	2.47349200	0.68726300
H	0.37406300	2.91261100	1.59012600
H	1.46152200	2.98774200	-0.90637300
C	1.77173200	-3.48444400	1.77979600
N	2.35239500	-4.46886100	1.96511700

#### BR2-CN-M4

Electronic energy: -708.78217 Hartree

Lowest frequency: 44.5098 cm<sup>-1</sup>

C	-2.57377800	0.82132500	-2.77510100
C	-2.49898900	0.82313300	-1.37813500
C	-1.34325900	1.29607700	-0.77940000
C	-0.26483100	1.74250200	-1.55319100
C	-0.32684700	1.72395500	-2.93715500
C	-1.50131000	1.26745900	-3.54454400
C	-0.96239100	1.39300600	0.69475900
C	1.64354100	0.84908500	-0.31829400
C	1.04918200	-0.12594900	0.52640200
C	-0.24626700	0.10491900	1.09166800
C	-0.81114300	-0.82928000	1.94707600



H	-1.79187300	-0.63588400	2.37294600
C	-0.14582500	-2.01224900	2.26123200
C	1.11609100	-2.25606700	1.69748400
C	1.70779100	-1.33278000	0.84151400
H	-3.47717700	0.47059500	-3.26425200
H	-3.33396200	0.46957200	-0.77948800
H	0.51053300	2.06479500	-3.53950500
H	-1.57797800	1.26151200	-4.62745200
H	-0.59057800	-2.74238000	2.92790300
H	2.68732100	-1.53644700	0.41960600
H	-1.80381500	1.59180900	1.36415100
H	2.59197100	0.64541600	-0.80396800
C	0.87985400	2.12594600	-0.61119600
C	0.09547300	2.46867700	0.63349100
H	0.56029300	2.88496400	1.52068900
H	1.53465000	2.91321200	-0.99106500
C	1.81109100	-3.47705600	2.01195800
N	2.36940400	-4.45883800	2.26583100

#### DBB\*-NO2-M1

Electronic energy: -820.97301 Hartree

Lowest frequency: 45.7428 cm<sup>-1</sup>

C	-2.81317100	1.56207100	-2.99846600
C	-2.78753700	1.59073000	-1.60166400
C	-1.57485200	1.46899300	-0.93974900
C	-0.38458200	1.31364200	-1.66876200
C	-0.40872600	1.29745900	-3.05686200
C	-1.63175700	1.41722900	-3.72070100
C	-1.37368800	1.48924800	0.56461400
C	0.85946200	1.24380400	-0.78704700
C	0.63369400	0.13042200	0.21619800
C	-0.57529500	0.24373100	0.92982900
C	-0.91394100	-0.69000400	1.90247800
H	-1.84265900	-0.59271500	2.45638000
C	-0.05909200	-1.76003600	2.15797200
C	1.12162800	-1.85359200	1.43431900
C	1.49371500	-0.92390400	0.46392400
H	-3.75976000	1.65374100	-3.52167700
H	-3.70815800	1.70862400	-1.03644400
H	0.51515800	1.18664300	-3.61810500
H	-1.65973600	1.39585000	-4.80566000
H	-0.29406300	-2.51302800	2.89979400
H	2.43131800	-1.03951000	-0.06727100
H	-2.30968100	1.55865600	1.12400600
H	1.77560100	1.11591000	-1.36827100

C	0.77588200	2.57832500	-0.04817200
C	-0.36538500	2.58367200	0.90830400
H	-0.16583000	2.71712200	1.97090000
H	0.94752900	3.45722800	-0.66832100
N	2.02168400	-2.98008600	1.70335400
O	1.69252400	-3.78139800	2.56073900
O	3.05108300	-3.05218700	1.05434200

### TS1-NO<sub>2</sub>-M1

Electronic energy: -820.95945 Hartree

Lowest frequency: -597.1266 cm<sup>-1</sup>

C	-0.01672200	0.21295500	-0.11482300
C	0.01039600	0.16630800	1.27963000
C	1.22217500	-0.01752500	1.93313900
C	2.40757300	-0.15537800	1.19924400
C	2.37932600	-0.10710900	-0.18842700
C	1.16162500	0.07677700	-0.84484500
C	1.39393900	-0.10269100	3.42671700
C	3.64835600	-0.33117600	2.05062000
C	3.42665500	-1.46747200	3.02946000
C	2.25787500	-1.27748600	3.82920300
C	2.01661100	-2.13214000	4.92880500
H	1.13101300	-1.98880700	5.54045500
C	2.88550100	-3.16561400	5.19724700
C	4.02270600	-3.33454900	4.38640900
C	4.31719600	-2.48146800	3.32318200
H	-0.96095800	0.35425400	-0.63109900
H	-0.90741200	0.27077500	1.85201200
H	3.30042500	-0.21264800	-0.75523500
H	1.13402300	0.11334200	-1.92932300
H	2.70995500	-3.85890400	6.01003200
H	5.22666100	-2.62579900	2.75133000
H	0.46766600	-0.03713300	3.99763900
H	4.55994300	-0.44198100	1.46175600
C	3.69396300	0.82163900	3.03735700
C	2.50399200	0.75981500	3.94017000
H	2.53894800	1.05376300	4.98121100
H	4.63458000	1.23182600	3.38300600
N	4.92914400	-4.42640900	4.67299700
O	4.67986200	-5.14507200	5.63221500
O	5.90321500	-4.57495700	3.94578600

### BR1-NO<sub>2</sub>-M1

Electronic energy: -820.9808 Hartree

Lowest frequency: 39.0107 cm<sup>-1</sup>

C	-2.74303700	1.28977000	-3.10357900
C	-2.78099100	1.28709800	-1.70874400
C	-1.59340000	1.33658800	-0.98632500
C	-0.36406200	1.37921000	-1.66401000
C	-0.32836300	1.38349000	-3.05134300
C	-1.52312600	1.33960200	-3.77253900
C	-1.53344700	1.35753700	0.49652800
C	0.85438300	1.42012900	-0.74716700
C	0.71766200	0.25065800	0.20560900
C	-0.34459800	0.59007600	1.15972700
C	-0.56779200	-0.31080600	2.27951800
H	-1.31823200	-0.06149100	3.02378000
C	0.14133300	-1.46980000	2.36465900
C	1.12300400	-1.77448100	1.38411500
C	1.43306000	-0.89663700	0.31295300
H	-3.66991700	1.25171900	-3.66691000
H	-3.73277200	1.24975200	-1.18569400
H	0.62678200	1.41602900	-3.56858300
H	-1.49847800	1.34001300	-4.85764200
H	-0.01659100	-2.17388400	3.17152700
H	2.23821900	-1.14887700	-0.36643400
H	-2.46896900	1.27912400	1.04297800
H	1.79364100	1.44690800	-1.30278400
C	0.63179600	2.57238500	0.21385000
C	-0.41915100	2.13192100	1.15864900
H	-0.63302800	2.66550700	2.07792300
H	0.79807200	3.60810200	-0.05503200
N	1.85571700	-2.99635100	1.50319900
O	1.60397800	-3.73760900	2.45173300
O	2.70430300	-3.24946400	0.64964800

### TS2-NO<sub>2</sub>-M1

Electronic energy: -820.97457 Hartree

Lowest frequency: -507.3711 cm<sup>-1</sup>

C	-2.45138600	0.88830600	-2.99505000
C	-2.55664000	0.96287500	-1.60916700
C	-1.40591600	1.10696100	-0.82674100
C	-0.13995900	1.12772400	-1.45405300
C	-0.04341700	1.05073100	-2.83453700
C	-1.20095700	0.93858800	-3.60876800
C	-1.44805200	1.21976100	0.62182900
C	1.04649100	1.17511200	-0.49502400
C	0.88785900	-0.03081400	0.41626100
C	-0.05910900	0.31444000	1.44003600

C	-0.42362400	-0.64783600	2.42179400
H	-1.10192000	-0.38398900	3.22709100
C	0.10442600	-1.91598400	2.33532000
C	1.00678200	-2.23035500	1.30429400
C	1.41098600	-1.28926800	0.33455600
H	-3.34827600	0.78949100	-3.59803900
H	-3.53111500	0.92805200	-1.12971600
H	0.93468000	1.06487100	-3.30805600
H	-1.12328800	0.87819000	-4.68957200
H	-0.14512800	-2.68022200	3.06050500
H	2.12273100	-1.57794300	-0.42979700
H	-2.37928700	1.04441300	1.15145200
H	1.99897700	1.22641600	-1.02693400
C	0.77251400	2.30854300	0.47140800
C	-0.29632600	1.80530800	1.38056600
H	-0.53355800	2.33822400	2.29788100
H	0.86438200	3.35096200	0.19151400
N	1.55793800	-3.56008000	1.24788300
O	1.20511600	-4.37228900	2.09626600
O	2.35466100	-3.81787400	0.35160000

### BR2-NO<sub>2</sub>-M1

Electronic energy: -820.99468 Hartree

Lowest frequency: 43.3958 cm<sup>-1</sup>

C	-2.50785700	1.36972400	-3.16988600
C	-2.67838100	1.63600800	-1.82210300
C	-1.56792800	1.70718700	-0.94790500
C	-0.26664000	1.47207200	-1.49257200
C	-0.11600200	1.21081000	-2.84496900
C	-1.22716300	1.15948700	-3.69012000
C	-1.71869800	2.00893800	0.43088300
C	0.91406200	1.49858700	-0.52226200
C	0.80132800	0.29083700	0.39946700
C	-0.01344800	0.62941200	1.49159400
C	-0.32223100	-0.30088100	2.47301900
H	-0.95609900	-0.04053400	3.31476000
C	0.21033600	-1.58601000	2.36921600
C	1.01299600	-1.89582000	1.27831500
C	1.32051900	-0.98206900	0.26857500
H	-3.37238000	1.32587400	-3.82486100
H	-3.67314700	1.80451500	-1.41804500
H	0.87983600	1.03880800	-3.24591200
H	-1.09464400	0.95251500	-4.74703900
H	0.01504200	-2.34363600	3.11771600
H	1.94636600	-1.27973000	-0.56446800

H	-2.70710500	2.11718200	0.86493400
H	1.86316000	1.56016200	-1.06113900
C	0.64296000	2.61295100	0.45933500
C	-0.48254400	2.07223700	1.31003100
H	-0.67207000	2.60403000	2.24489100
H	0.71300400	3.66027200	0.18729400
N	1.56876700	-3.25023400	1.18388000
O	1.28422800	-4.04774800	2.06078100
O	2.28570100	-3.50482600	0.23117500

### DBB\*-OCH<sub>3</sub>-M1

Electronic energy: -731.02053 Hartree

Lowest frequency: 44.4601 cm<sup>-1</sup>

C	-2.69191400	1.02543400	-2.99825500
C	-2.66942400	1.15198100	-1.60640300
C	-1.45438100	1.14318600	-0.93787200
C	-0.25534100	1.00475500	-1.65795700
C	-0.27703100	0.89265400	-3.04160800
C	-1.50322700	0.89752200	-3.71111000
C	-1.25388000	1.27474800	0.56046300
C	0.98963100	1.06407100	-0.77660300
C	0.82841200	0.00703200	0.29993100
C	-0.38675900	0.10158700	1.00595800
C	-0.65360000	-0.79030400	2.02963500
H	-1.58337000	-0.71923300	2.58809600
C	0.26623500	-1.79598800	2.35042100
C	1.46175700	-1.88860600	1.63872600
C	1.74497100	-0.97748600	0.60825800
H	-3.64152700	1.02816700	-3.52438800
H	-3.59660400	1.25779400	-1.04913100
H	0.65304000	0.79569500	-3.59562100
H	-1.52753800	0.80017700	-4.79217800
H	0.03650300	-2.49198900	3.14820300
H	2.68649700	-1.06965800	0.07493300
H	-2.19431900	1.32917800	1.11519900
H	1.91102300	0.95214300	-1.35373600
C	0.82858900	2.43950200	-0.13241300
C	-0.31602800	2.45216900	0.82093100
H	-0.11989100	2.65883300	1.87290000
H	0.95574000	3.28178000	-0.81226000
O	2.42091100	-2.82592300	1.86686900
C	2.17979600	-3.76765500	2.89110200
H	1.28201400	-4.36123200	2.68212800
H	3.05068000	-4.42230000	2.91235800
H	2.06890700	-3.27641100	3.86500900

**TS1-OCH<sub>3</sub>-M1**

Electronic energy: -731.00024 Hartree

Lowest frequency: -600.5694 cm<sup>-1</sup>

C	-0.02965800	-0.00309400	-0.16148500
C	-0.01397100	0.02394900	1.23371600
C	1.19883500	-0.03814900	1.90936900
C	2.40017700	-0.13158900	1.19249500
C	2.38229100	-0.15942000	-0.19620300
C	1.16374700	-0.09440800	-0.87355800
C	1.35431100	-0.03473900	3.40296400
C	3.64168300	-0.18487900	2.05728600
C	3.49009800	-1.28637700	3.08238700
C	2.32081200	-1.08124600	3.89420100
C	2.14588300	-1.89539900	5.04087100
H	1.26068700	-1.77157900	5.65844900
C	3.08168900	-2.85785300	5.36467800
C	4.22670700	-3.03953600	4.55897100
C	4.43057400	-2.23288500	3.43255100
H	-0.97567400	0.04662400	-0.69178200
H	-0.94371900	0.09376700	1.79252300
H	3.31553500	-0.23086900	-0.74893100
H	1.14741500	-0.11516200	-1.95893200
H	2.91790900	-3.48197200	6.23547900
H	5.33598000	-2.37120600	2.84868400
H	0.41815200	-0.00729500	3.96072000
H	4.56215100	-0.25569300	1.47496600
C	3.60295300	1.00662500	3.00647300
C	2.42432700	0.88462000	3.91147900
H	2.40090800	1.25857100	4.92538700
H	4.52842200	1.43785400	3.37171800
O	5.18825600	-3.97177300	4.80162700
C	5.02117000	-4.81142900	5.92434400
H	4.10499900	-5.40811400	5.84326500
H	5.88512300	-5.47553300	5.93694400
H	4.99404100	-4.23257300	6.85516900

**BR1-OCH<sub>3</sub>-M1**

Electronic energy: -731.01936 Hartree

Lowest frequency: 40.1574 cm<sup>-1</sup>

C	-2.63517600	0.78701000	-3.09277700
C	-2.66637900	0.87012300	-1.70077400
C	-1.48123700	1.01936800	-0.98523600
C	-0.25605900	1.07175900	-1.67470900

C	-0.22847700	0.98940000	-3.06075100
C	-1.42101500	0.84896500	-3.77239400
C	-1.41364600	1.11885300	0.49056700
C	0.96504000	1.21535500	-0.77366700
C	0.88219200	0.09377400	0.24079000
C	-0.19116300	0.45887800	1.18932600
C	-0.34163500	-0.39808300	2.36347400
H	-1.07254900	-0.13711800	3.12281600
C	0.41246400	-1.53924600	2.48334900
C	1.38108800	-1.88293100	1.51316900
C	1.62502600	-1.02569000	0.39906400
H	-3.56232200	0.67500400	-3.64644700
H	-3.61400100	0.82289800	-1.17034000
H	0.72310300	1.03219400	-3.58475400
H	-1.40027000	0.78578900	-4.85599700
H	0.26385400	-2.17656900	3.34804400
H	2.42897100	-1.28566800	-0.28383600
H	-2.34596400	1.05586000	1.04550100
H	1.89644400	1.25196900	-1.34360900
C	0.70104200	2.41334300	0.12100400
C	-0.31438100	1.98299700	1.10449500
H	-0.56013600	2.57603100	1.97841900
H	0.80658200	3.43419700	-0.22716000
O	2.16219400	-2.99348800	1.56483200
C	1.98688600	-3.87024800	2.65780700
H	0.96574100	-4.26811800	2.68727400
H	2.69091700	-4.68822900	2.50722800
H	2.20733900	-3.36961800	3.60797100

### TS2-OCH<sub>3</sub>-M1

Electronic energy: -731.01445 Hartree

Lowest frequency: -558.03 cm<sup>-1</sup>

C	-2.42152500	0.62955200	-2.96860400
C	-2.53421500	0.74850000	-1.58662800
C	-1.40787800	1.04215300	-0.80906400
C	-0.15201800	1.17080100	-1.44591200
C	-0.04794800	1.04919200	-2.82409600
C	-1.18376700	0.78633700	-3.59201800
C	-1.44937700	1.18259100	0.63838400
C	1.02388300	1.38245500	-0.49723700
C	0.99178700	0.20121100	0.45616200
C	-0.00951000	0.48211400	1.45889700
C	-0.21892500	-0.47497600	2.49398500
H	-0.90796000	-0.26203000	3.30577300
C	0.45309100	-1.68484700	2.44956000

C	1.37880900	-1.95750300	1.42694800
C	1.65072300	-0.99246300	0.42677900
H	-3.30453800	0.41531400	-3.56301900
H	-3.50082300	0.62987800	-1.10375700
H	0.92463100	1.15080900	-3.29964500
H	-1.10065300	0.69615500	-4.67052400
H	0.27269400	-2.41334200	3.23156400
H	2.39344000	-1.22525800	-0.33076200
H	-2.36570600	0.95981300	1.17600800
H	1.96435200	1.51357400	-1.03827900
C	0.63652100	2.51699100	0.42999500
C	-0.36962500	1.94228300	1.36463200
H	-0.66207300	2.48753400	2.25827400
H	0.61545800	3.54994400	0.10216700
O	2.08492200	-3.11478700	1.31993700
C	1.86224900	-4.11088200	2.29531400
H	0.81613300	-4.43905200	2.29593900
H	2.50527000	-4.94849600	2.02628400
H	2.12912200	-3.75350900	3.29693400

### BR2-OCH<sub>3</sub>-M1

Electronic energy: -731.04157 Hartree

Lowest frequency: 43.7118cm<sup>-1</sup>

C	-2.47595700	0.78779900	-3.18710800
C	-2.67958400	1.07897900	-1.84877500
C	-1.58811200	1.29397900	-0.97423700
C	-0.26584500	1.17822500	-1.50876400
C	-0.08359600	0.89111600	-2.85225700
C	-1.17807700	0.69563400	-3.69833800
C	-1.77565200	1.62401300	0.39397200
C	0.90215100	1.36170400	-0.54026900
C	0.92599500	0.17950700	0.42207900
C	0.07610000	0.46280800	1.50294400
C	-0.11116200	-0.47377200	2.50030900
H	-0.77025800	-0.27349600	3.34064800
C	0.57002000	-1.69749000	2.43393700
C	1.41250200	-1.96990300	1.35500100
C	1.58825800	-1.02571900	0.32882500
H	-3.32837100	0.63230600	-3.84132900
H	-3.68892200	1.15596300	-1.45260900
H	0.92732900	0.81167000	-3.24495500
H	-1.01899700	0.46907000	-4.74772200
H	0.43528800	-2.42178200	3.22821000
H	2.24539200	-1.26866600	-0.50079400
H	-2.77349500	1.64015800	0.82052000



H	1.83851600	1.51289100	-1.08481300
C	0.50559400	2.47187700	0.40353300
C	-0.55648500	1.83704400	1.27182600
H	-0.80399900	2.38045300	2.18693700
H	0.45431000	3.50949700	0.09021900
O	2.11503500	-3.12640000	1.20614800
C	1.96884800	-4.11159900	2.20665300
H	0.92822400	-4.44801800	2.28478400
H	2.59844300	-4.94778900	1.90341200
H	2.30166900	-3.73991800	3.18306000